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Examiner copy
reference #2**A Primer on Mass Spectrometers**

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The mass spectrometer is simply a detector. With this detector we can simultaneously gather both qualitative (identity) and quantitative (amount) information about chemical compounds or elements. At Manchester, mass spectrometers are used for the analysis of both elements (ICP/MS) and organic compounds (GC/MS). Elemental analysis on the ICP/MS in Region 10 applies almost exclusively to metals analysis.

Before the sample can be introduced to the instrument the analytes of interest must be separated from the matrix using acid digestion for elemental analysis or solvent extraction for organics analysis. Once the sample is prepared and presented to the instrument, the analytical tool is basically the same.

A mass spectrometer consists of several parts: a means to introduce the sample (inlet); a means and place to produce charged fragments or ions (ion source); a mass filter (ion analyzer) which "sorts" the ions; an ion detector.

Inlet - In elemental analysis, the inlet is also the ion source, as described in Maricia Alforque's article on ICP/MS in the last newsletter. A peristaltic pump introduces the sample solution to the argon plasma which produces highly excited elemental ions ready for the mass filter.

For organic analysis gas chromatography (GC) is used to separate compounds in a mixture before introduction into the ion source. After GC, all molecules of each unique compound enter the ion source within a relatively narrow time window and are separated by time from other compounds. **Ion Source** - Organic analysis requires that the compounds maintain their integrity until charged molecules are produced and so requires a less energetic ionization than an argon plasma. At Manchester charged molecules are produced by electron impact. Electrons are produced in the source from a glowing filament and focused into an electron beam by accelerating them toward an anode through a slit, sort of like an electron gun. A very small portion of the organic molecules enter the source from the gas chromatograph, diffuse through the beam, are influenced by the electrons and form ions. While both positive and negative organic ion fragments are formed, normally only positive ions are counted. Positive ions tend to give more fragmentation, and thus structural information on organic compounds. ICP/MS also analyzes positive ions as these are what are produced in the plasma. Positive ions are drawn toward the mass filter and focused into a well defined ribbon or column for entry into the

mass filter.

Ion Analyzer - A mass filter separates ions by the combination of the charge on the ion and its mass. Although there are several ways to do this, environmental analysis generally uses the quadrupole mass filter.

A quadrupole consists of four parallel, equidistant charged rods. As an ion heads down the space between the rods, two opposite rods are charged positive and the remaining two negative. A positive ion will be attracted toward the closest negative rod. The rod polarity switches after a time changing the ion's path toward the new closest negative rod. Polarity is switched regularly at a predetermined frequency all during the flight of the ion down the quadrupole. If an ion is lighter than the mass targeted it will hit a negatively charged rod before it changes polarity. If it is too heavy eventually it won't have moved far enough away from a positively charged rod to avoid crashing when it becomes negative. Only if the frequency of the switching is exactly right for the mass of interest will the ion be able to spiral along the length of the quadrupole without hitting a rod. By altering the voltage or frequency on the rods, the mass of the ion which can succeed changes. A scanning quadrupole mass spectrometer sweeps through the masses of interest by this means.

Ion Detector - After an ion has successfully run the quadrupole gauntlet it strikes the electron multiplier (EM) causing electrons to eject. The surface geometry of the EM is arranged such that each electron from the initial collision hits the surface repetitively, ejecting more electrons each time an electron strikes the side of the EM. This "ion multiplier" increases the total number of electrons ejected per ion making it through the quadrupole. The detected signal is a voltage caused by the number of electrons ejected which is proportional to the number of ions which made it down the rods at the particular voltage/frequency combination representing a particular mass.

During elemental MS analysis all analytes are introduced into the spectrometer at the same time in a constant stream of sample elemental ions. The MS repeatedly scans over the mass range and develops one signal for each elemental isotope detected.

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→ During organic mass spectrometry several fragments are produced for each compound analyzed. Imagine dropping a Lego model. The model might break apart, perhaps in several pieces. Dropping an identical model might produce some of the same pieces, or different ones. The pieces produced after many such experiments could be counted to determine where the model was most likely to fragment, where the bonds were weakest. Billions, trillions, or more molecules enter the ionization chamber of a mass spectrometer at a time and later fragment. Like the model, the population of each of the fragments produced reflects the internal structure of the molecule. The bar chart of a fragment population versus mass is called a mass spectrum. A mass spectrum is reproducible for any compound given approximately the same instrument parameters because the structure of the molecule determines the probability of fragment formation. Because organic mass spectra are relatively stable from instrument to instrument, the information can be stored in a data base (a mass spectrum library) and unknown spectra searched against it. The Manchester lab's most current organic mass spectrum library is from The National Institute for Standards and

Technology and consists of more than 75,000 spectra. For all its complexity, the mass spectrometer is remarkably reliable and accurate and is a mainstay of Region 10's analytical arsenal.

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